

Erratum: "IUPAC-NIST Solubility Data Series. 80. Gaseous Fluorides of Boron, Nitrogen, Sulfur, Carbon, and Silicon and Solid Xenon Fluorides in all Solvents"
[J. Phys. Chem. Ref. Data 34, 201 (2005)]

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[1] The following page numbers are incorrect: Page 203, last paragraph, page 019 should be page 215; page 020 should be page 216; page 050 should be page 232.

[2] Page 203, column 1, last paragraph: Figures on p. 215 are from the *Journal of the American Chemical Society*, not the *Journal of Physical Chemistry*.

[3] Page 202, right-hand column and p. 227, right side, Table 7: Table 7 is misplaced. Instead of being on the second page of the evaluation under 3.4. (OC-6-11)-Sulfur Fluoride, it should be on p. 228, right side. Table 7 title and caption on pp. 202 and 227, respectively, should read "Smoothed tentative values of the mole fraction solubility of SF₆ in H₂O at 0.101325. . ."

[4] Page 202, right-hand column and p. 238, left side, Table 8: The heading above authors should be Evaluators, not Original Measurements. Table 8 title and caption on pp. 202 and 238, respectively, should read, "The tentative mole fraction solubility of SF₆ in H₂O-*d*2 at a partial pressure. . ."

[5] Page 202, right column. The title for Table 10 should be: "Smoothed tentative values of the mole fraction solubility of CF₄ in D₂O at 0.101325 MPa."

[6] Page 331, right-hand column, the experimental data discussed is for 1,1difluoroethane or HFC-152a—this discussion should have appeared in Sec. 3.14.

[7] Page 338, Fig. 3 is the wrong figure; this entire evaluation is repeated in the following section (Sec. 3.8) with the correct figure.

[8] Page 393, Fig. 4 is the wrong figure; this entire evaluation is repeated in the following section (Sec. 3.17) with the correct figure.

[9] Pages 420-435, the System Index, Registry Number Index, and Author Index: For all page numbers subtract 1 to get the proper page reference.

[10] Page 427, for the System Index entry uranium hexafluoride + xenon fluoride, XeF₂, add ",213."

[11] Page 428, for the System Index entry water-*d*2 + methane, tetrafluoro, the page number should be E295 not E205.

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3.8. Fluoromethane

Components:

- (1) Fluoromethane; CH₃F; [593-53-3]
(2) Water; H₂O; [7732-16-5]

Evaluation:

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Evaluation

An evaluation of the solubility of fluoromethane in water at a partial pressure of 0.101325 MPa from 273.15 K to 353.15 K.

Three papers report the solubility of fluoromethane in water. Glew and Moelwyn-Hughes¹ report nine values between 273.21 K and 353.40 K. Henry's law was tested at 303.15 K and maybe other temperatures as well. This is a complete and careful study. Swain and Thornton² report eight values, four near 302.6 K and four near 313.5 K. Rosenthal and Nickels³ report one value at 310.15 K using a radioactive isotope method.

The 18 experimental values of the mole fraction solubility of fluoromethane in water were fit by a non-linear regression to the three constant Clark, Glew, and Weiss (CGW) equation and to the three constant Benson and Krause equation (BK). After elimination of the 283.15 K value from Glew and Moelwyn-Hughes¹ and the 315.15 K value of Rosenthal and Nickels³ very satisfactory fits were obtained to the 16 remaining values with both equations. Both equations are given here, but the CGW equation was chosen to calculate the recommended smoothed value of mole fraction solubility at 0.101325 MPa partial pressure, the Ostwald coefficients, and the thermodynamic changes on solution in table.

The CGW equation is:

$$\ln x_1 = -(50.4960 \pm 1.7111) + (73.5668 \pm 2.4905)/(T/100 \text{ K}) + (17.3725 \pm 0.9017)\ln(T/100 \text{ K}),$$

where x_1 is the mole fraction solubility of CH₃F at a partial pressure of 0.101325 MPa and $(T/100 \text{ K})$ is the Kelvin temperature divided by 100 K. Ostwald coefficients and thermodynamic changes on solution were also calculated and they are given in the Table below at five degree intervals from 273.15 K to 353.15 K. The fit $r^2 = 0.9995$ with a standard error of the fit of 0.0085.

The BK equation is:

$$\ln x_1 = -(4.7796 \pm 0.4366) - (3393.3505 \pm 269.6518)(T/K)^{-1} + (828076.0404 \pm 41.614)(T/K)^{-2},$$

where x_1 is the mole fraction solubility of CH₃F in water at a partial pressure of 0.101325 MPa and T is the Kelvin temperature. The fit $r^2 = 0.9994$ with a standard error of the fit of 0.0092.

The values are given in Table 11 and Fig. 3.

References

- ¹D. N. Glew and E. A. Moelwyn-Hughes, Disc. Faraday Soc. **15**, 150–161 (1953).
²C. G. Swain and E. R. Thornton, J. Am. Chem. Soc. **84**, 822–826 (1962).
³M. S. Rosenthal and R. J. Nickels, Phys. Med. Biol. **30**, 945–950 (1985).

TABLE 11. The recommended mole fraction solubility of fluoromethane in water at a partial pressure of 0.101325 MPa and at five degree intervals from 273.15 K to 353.15 K. Also given are values of the Ostwald coefficient and the thermodynamic changes on solution.

Temperature	Mole fraction	Ostwald Coefficient	Enthalpy changes	Entropy changes	Heat capacity change
T/K	$10^3 x_1$	$L/\text{cm}^3 \text{ cm}^{-3}$	$\Delta_{\text{sln}} H^\circ/\text{kJ mol}^{-1}$	$\Delta_{\text{sln}} S^\circ/\text{J K}^{-1} \text{ mol}^{-1}$	$\Delta_{\text{sln}} C_p/\text{J K}^{-1} \text{ mol}^{-1}$
273.15	2.228	2.78 ₀	-21.71	-130.3	144
278.15	1.882	2.39 ₀	-20.94	-127.6	144
283.15	1.608	2.06 ₅	-20.27	-125.1	144
288.15	1.388	1.82 ₀	-19.54	-122.5	144
293.15	1.211	1.61 ₅	-18.82	-120.0	144
298.15	1.067	1.44 ₅	-18.10	-117.6	144
303.15	0.948	1.30 ₅	-17.38	-115.2	144
308.15	0.849	1.18 ₅	-16.66	-112.8	144
313.15	0.767	1.08 ₅	-15.94	-110.5	144
318.15	0.699	1.00 ₅	-15.21	-108.2	144
323.15	0.640	0.93 ₀	-14.49	-106.0	144
328.15	0.591	0.87 ₀	-13.77	-103.8	144
333.15	0.549	0.82 ₀	-13.05	-101.6	144
338.15	0.513	0.77 ₅	-12.33	-99.4	144
343.15	0.482	0.73 ₅	-11.60	-97.3	144
348.15	0.456	0.70 ₅	-10.88	-95.2	144
353.15	0.433	0.67 ₅	-10.16	-93.2	144

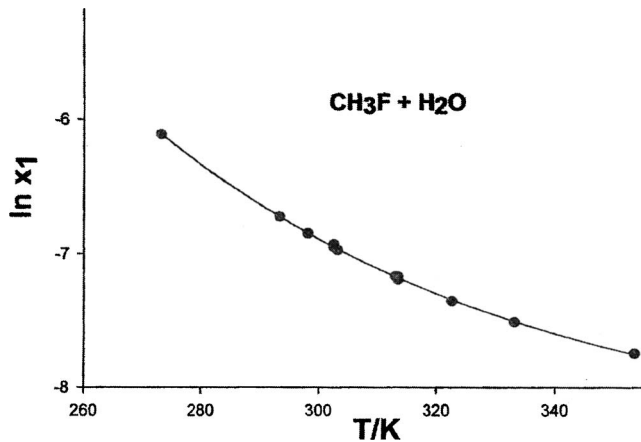


FIG. 3. The solubility of fluoromethane in water. $\ln x_1$ vs. T/K . The fitted line and experimental points.

3.17. Octafluorocyclobutane

Components:

(1) Octafluorocyclobutane; $c\text{-C}_4\text{F}_8$; [115-18-5]
 (2) Water; H_2O ; [7732-18-5]

Evaluators:

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Evaluation

Evaluation of the solubility of octafluorocyclobutane in water at a partial pressure of 0.101325 MPa between 278.15 K and 318.15 K. Four papers report on the solubility of octafluorocyclobutane in water. Two of the papers are from the same laboratory. Filatkin *et al.*¹ do not report their data, but give a fitted equation, which requires knowledge of the gas critical constants. The compiler calculated solubility values at three temperatures from the author's equation. The mole fraction and Ostwald coefficient values are a factor of ten larger than the values in the other three papers. There is doubt about these values and they are rejected for the present. Efforts to clarify the doubts about this paper are under way, but may not succeed before this goes to print.

Wen and Muccitelli² report six values of the solubility between 278.15 K and 303.15 K at a partial pressure of 0.10133 MPa. There are two papers from the laboratory of R. Battino: Park *et al.*³ report one value of the solubility at 298.15 K and 0.10133 MPa and Scharlin and Battino⁴ report four values from 288.22 K to 318.23 K and 0.10133 MPa partial pressure. The 298.15 K mole fraction solubility from the three papers is 2.20, 2.17, and 2.37×10^{-6} . The average is $(2.24 \pm 0.11) \times 10^{-6}$. The eleven experimental values from the three papers were treated by a non-linear regression to obtain the CGW and BK equations with three constants each. All of the eleven values fell within two standard deviations of the equations. The results are:

CGW Equation.

$$\ln x_1 = -(196.5062 \pm 35.7101) + (277.2389 \pm 50.7444)/(T/100 \text{ K}) + (82.8621 \pm 17.1014)\ln(T/100 \text{ K}).$$

with $r^2 = 0.9855$ and the standard error of estimate 0.0474 in $\ln x_1$. The temperature of minimum solubility is 334.6 K according to the equation.

BK Equation.

$$\ln x_1 = (18.1746 \pm 8.6360) - (21,580 \pm 5,118.8360)(1/(T/K))^{-1} + (3663004 \pm 758625)(1/(T/K))^{-2}$$

with $r^2 = 0.9984$ and the standard error of estimate 0.0475 in $\ln x_1$.

The CGW equation is used to construct Table 13 and Fig. 4.

References

¹V. N. Filatkin, V. T. Plotnikov, and A. G. Alishev, Kholod. Tekh. (No. 2), 23–25 (1976).

²W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. 8, 225–246 (1979).

³T. Park, T. R. Rettich, R. Battino, D. Peterson, and E. Wilhelm, J. Chem. Eng. Data 27, 324–326 (1982).

⁴P. Scharlin and R. Battino, Fluid Phase Equilibrium 94, 137–147 (1994).

TABLE 13. The tentative mole fraction solubility of octafluorocyclobutane in water from 278.15 K to 318.15 K at a partial pressure of 0.10133 MPa. Also values of the Ostwald coefficient and thermodynamic changes on solution.

Temperature T/K	Mol Fraction $10^6 x_1$	Ostwald Coefficient $L/\text{cm}^3 \text{ cm}^{-3}$	Enthalpy Change $\Delta_{\text{sln}} H^\circ/\text{kJ mol}^{-1}$	Entropy Change $\Delta_{\text{sln}} S^\circ/\text{J K}^{-1} \text{ mol}^{-1}$	Heat Capacity Change $\Delta_{\text{sln}} C_p^\circ/\text{J K}^{-1} \text{ mol}^{-1}$
278.15	5.748	0.728	-38.92	-240.1	689
283.15	4.328	0.588	-35.43	-228.3	689
288.15	3.376	0.443	-31.99	-215.8	689
293.15	2.721	0.363	-28.54	-203.9	689
298.15	2.226	0.301	-25.10	-192.2	689
303.15	1.937	0.266	-21.65	-180.8	689
308.15	1.703	0.238	-18.21	-169.5	689
313.15	1.537	0.218	-14.76	-158.4	689
318.15	1.420	0.204	-11.32	-147.5	689

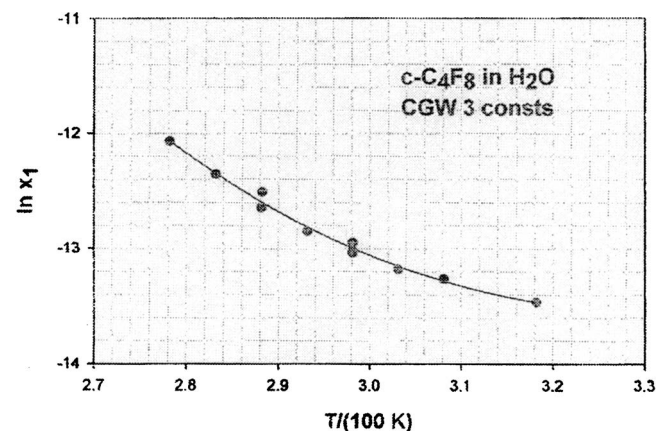


FIG. 4. The solubility of octafluorocyclobutane in water: $\ln x_1$ vs. $T/(100 \text{ K})$. The fitted curve and experimental points.